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Summary for the

Defense University Research Instrumentation Program

Equipment for High Performance Computing, Quantification and Visualization

DURIP CONTRACT: F49620-97-1-0251 DOLLAR AMOUNT = \$113,138.00 Rutgers The State University of New Jersey Piscataway, NJ, September 1998

1 Executive Summary

The equipment purchased under this grant was primarily dedicated to upgrading the visualization- simulation environment in our laboratory (our SGI machines, which are the main workstations being used for this task) to increase the turn-around time for studying complex simulations. The equipment included: SGI ONYX2 upgrade and Memory \$77,000, Boxhill Disk Systems \$28,000, and some memory and switch equipment \$8,000. Our laboratory, The Laboratory for Visiometrics and Modeling, CAIP Center, is an interdisciplinary laboratory with research focuses in both Computational Fluid Dynamics (CFD) and Visualization. Researchers in the laboratory come from both disciplines and work closely together.

The CFD simulations we generate are currently on the order of 256³ (and higher) vorticity datasets with 100-1000 timesteps per run. The area of research is turbulence and in particular accelerated inhomogeneous flows. The long-time simulations are necessary to capture and maintain high gradient phenomena associated with shock waves, contact discontinuities, shear layers, turbulence and mixing. The results of many of these simulations have not been thoroughly understood from a vortex-coherent structure viewpoint. This has resulted from the inadequate visualization and quantification of such massive datasets.

We have developed a sophisticated software environment that has enabled us to extract and track 3D time varying features from large structured and unstructured simulations and then visualize the evolution of these features individually. Quantifications such as volume change over time and feature cardinality change are also computed. This type of analysis and visualization is the only way one can cogently assimilate large continuum simulations. The equipment purchased under this grant has allowed us to attain interactive speeds of our feature tracking software for datasets with up to 1000 timesteps (structured and unstructured) and to experiment with integrating the visualization within the computations. Our future work involves distributing the visualization computations and using the same data structures for both the computation and visualization.

2 Research Thrust

The equipment we purchased under this grant addressed the Computational Fluid dynamics and Computational Plasma Physics of the CFP, and the post-processing of the large time varying datasets which results from these simulations. Our specific research thrusts lie in following areas:

- Computational Fluid Dynamics (CFD) of compressible and shock driven flows,
- Visualization to support the extraction and tracking of features that appear in our simulations for reduced modeling, and
- Parallel computations, in both CFD and Visualization.

Our laboratory (The Laboratory for Visiometrics and Modeling) is unique in that it is truly multidisciplinary. (The PI's of the laboratory are Prof. Norman Zabusky, Department of Mechanical and Aerospace Engineering, and Prof. Deborah Silver, Department of Electrical and Computer Engineering.) Students from both CFD and Computer Graphics work in the same facility side by side. The research results enabled by the equipment purchase are described below.

3 CFD

Scientific investigations into the nature of accelerated inhomogeneous flows have a direct bearing on DOD missions. This environment, called the Rayleigh-Taylor (RT; incompressible flows) or Richtmyer-Meshkov (RM; compressible flows), manifests itself in a variety of situations, some of which are of military interest. Imploding cavities are the fundamental mechanism behind cavitation and microjets (of interest to the Navy), while shock-accelerated density interface cause the Munroe effect in shaped charges (Army). Shock-induced mixing of fuel bubbles in air has been proposed as a mechanism fuel-air mixing in SCRAMJET engines (Air Force). RM flows are dominated by the creation and evolution of coherent vortex structures, and we proposed the vortex paradigm [HZ89]. "Vortex dynamics" deals with the motion of fluids at high Reynolds number that are dominated by localized concentrations of vorticity (or coherent vortex structures) embedded in a nearly passive-incoherent background (or sea) of intermixed and distributed vorticity. Apart from fluid dynamics, we also have experience in re-entry wakes and the fluid dynamics of radar backscatter from vortex driven turbulent mediate and high altitude nuclear effects [Zab77, ZK65, ZDIP73, Zab84].

Our focus is on the Richtmyer-Meshkov (RM) and Rayleigh-Taylor (RT) environments in two and three dimensions with Euler and Navier-stokes codes. In the last year we have found the appearance of "vortex projectiles" (VPs) to be a common occurrence in the presence of closed topologies. In the compressible domain, we have investigated the interactions between shocks and bubble-like geometries (e. g. circular cylinder, sphere, ellipse and ellipsoid) with particular attention to the structure of the circulation deposited and the deformation rate of the interface. Of interest is the departure (separation) of vortex layers from the interface and the formation of projectiles, as these processes affect mixing with the ambient medium. Visualization and quantification is used to develop vortex paradigms to quantify the circulation magnitudes and structures and growth rate of the mixing layer. This requires a detailed study of shock dynamics (reflection/refraction/transmission) at interfaces and the formation of shear layers at multitudes of triple points.

Another approach involved developing a semi-Lagrangian incompressible numerical algorithm capable of preserving sharp interfaces during a long time of computation. It is based on the CASL code of Dritschel [DA97] and the work of Trygvasson [Try98]. We have addressed the sinusoidal and planar interface excited by one and then two ("reacceleration") impulses of varying duration. The possible factors affecting the limiting descriptors of the vorticity as it localizes include growth rate of amplitude, centroid and moments, rate of strain on the interface and baroclinic sources. Comparisons with the Jacobs and Niederhaus [JN98] data are ongoing.

Our objectives are three-fold (a) to employ sophisticated physics in our codes (specifically chemistry and radiation effects) and (2) to incorporate Adaptive Mesh Refinement techniques [BC89] and (3) to visualize and quantify the resultant data to understand the result and allow us to build predictive models. We are currently writing AMR code in the DAGH environment (http://www.caip. rutgers.edu/~parashar/DAGH/) and will incorporate advanced data-encapsulation and object-oriented techniques. We conjecture that the reduction of speed due to OOP and AMR overheads will be more than compensated by the sparser grid. For the impulsive acceleration problem, we applied an incompressible semi-Lagrangian numerical algorithm based on the Contour Advection Semi-Lagrangian (CASL) algorithm [DA97] modified with the vortex-in-cell technique [Try98] for ideal flows with vortex sheets and density interfaces. The interfaces are tracked by nodes (tracers) advecting with velocity of the flow field computed on 128×128 Eulerian mesh. Time integration employs the 4-th order Runge-Kutta method with an adaptive time step. To prevent instant roll-ups, the node redistribution procedure [DA97] is invoked every other time step. The code has been run on the upgraded

¹A vortex projectile (VP) is a localized configuration of positive and negative vorticity whose centroid rotates about a point that is remote from the configuration. Its simplest form is the translating rectilinear pair of opposite circulation line vortices in 2D.

compute engine in our laboratory.

We have also implemented a volume tracking algorithm (described Section 4) using a template matching routine to extract features from time-evolving vortex dynamics data sets and track them through their lifetime [SW97]. This was employed successfully in examining shock-titled ellipse interactions [ZR98]. Escaping vortex projectile were identified and tracked, gathering data on their strength and shape as they move away from their site of formation. A sample result is shown in Fig. 1. The full results are posted on the Web at http://vizlab.rutgers.edu/~jaray/FeatureTrack/ShockEllipseViz.html

A more sophisticated approach to visualization and analysis of the simulation data is being developed. We plan to use a SMP-MPP configuration to form an integrated simulation-diagnostics environment. While our production codes have been parallelized, many visualization/post-processing algorithms do not admit data locality (and a few are inherently serial) making it necessary to execute them on a shared-memory computer with a few but very fast processors. A coupled SMP-MPP configuration provides all the requirement for a hybrid simulation-diagnostic environment. Adaptive grids are expected to provide challenges to visualization due to the more involved data storage and representation schemes. While coherent fluid structures are expected to be "crisper", the requirements for sophisticated data structures to store, segment and track the different objects are expected to be more stringent. By any yardstick, tracking multiple objects in a 10⁶ point grid over 5000 time-steps is no trivial matter and we expect new issues to surface with time.

4 Volume Tracking

We have developed a sophisticated visualization/quantification environment which allows us to observe and follow phenomena of interest in both 2D and 3D time-varying datasets [SSZC94, SW97]. In this algorithm, connected regions are extracted from one dataset and then matched in subsequent datasets (what results is a tracked isosurface). The algorithm classifies events for each feature as one of Continuation, Creation, Dissipation. Bifurcation and Amalgamation by determining the best overlap for a feature in the next timestep. All features are tracked, as well as the mass, the moments and the volume change of these features. However, any type of connected component feature can utilize the tracking algorithm (e.g., cores [BS95], etc.). We have recently extended the algorithm to handle unstructured grids. The algorithm can be run real-time on the upgraded hardware in our laboratory, allowing us to experiment with different feature definitions for tracking.

A 2D example of tracking related to the CFD described above is shown in Fig. refshock.

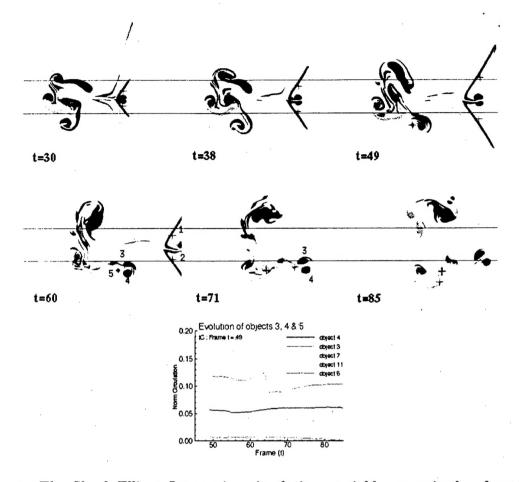


Figure 1: The Shock-Ellipse Interaction simulation, variable=magnitude of vorticity, 2D: 1024x640. Feature Tracked dataset. Below, quantification (circulation of objects 3,4 and 5).

The physical picture is that of a shock translating through space and hitting a prolate elliptical bubble of gas (in our case, heavier than ambient) angled at alpha to the vertical. The interaction deposits circulation on the interface and fragments the bubble as well. Using a 10 dynamical processes. Objects are colored according to the sign of their circulation (note: magnitude does not influence the color) blue for negative circulation and yellow to red for positive. As the simulation proceeds the fragments (patches of vorticity) interact (merge or split) and we track their evolution.

A 3D example is shown in Fig. 2. Fig. 2(a) results from a compressible simulation in the HSCT (High Speed Civil Transport) inlet unstart configurations [ZKSH97]. To work with high cruise efficiency, the HSCT inlet is designed to work under the so called "critical operation". The critical operation locates a terminal shock just downstream of the throat to maintain high total pressure recovery with the maximum mass flow.

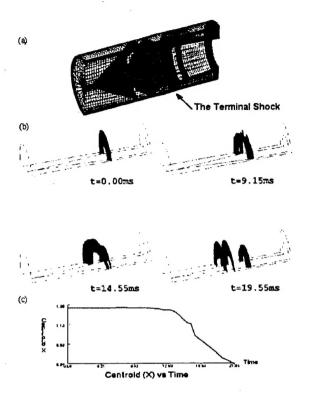


Figure 2: HSCT Simulation: Simulation of shock vortex features in compressible inlet unstart configurations. (a)Mesh and shocks are shown. (b) The terminal shock is tracked (c) The x coordinate of the centroid position of the terminal shock is computed over time.

However, the terminal shock location is very sensitive to disturbance and can be pushed out of the inlet to cause the inlet unstart. The inlet unstart will introduce instability to the whole aircraft and may also cause engine surge. This simulation is performed on a curvilinear grid, which is 72 points in the streamwise direction, 16 points in the circumferential direction and 42 points in the radius direction. The mesh and shocks segmented from the pressure gradient are shown in Fig. 2. Fifty two time steps were used for tracking. The tracking was done in the computational domain and the results were mapped to the physical domain for visualization. (This simulation was provided courtesy of Prof. Doyle Knight, and Dr. Gecheng Zha, Dept. of Mechanical and Aerospace Engineering, Rutgers University.)

Other examples applied to weather, oceanographic and numerous simulations can be seen on our web site http://www.caip.rutgers.edu/vizlab.html. Feature tracking modules for AVS, Vis5D, and Vtk are also available on our web site.

Our future efforts in this area involve developing an interactive user interface to the tracking code (possible because of the high powered compute engine upgraded as part

of this durip) and distributed the visualization code with the simulation code using the DAGH data structure described above.

5 Research Publications

The laboratory has produced a number of publications in both CFD and Visualization using the equipment and enhancements purchased under this grant during 1997 and 1998. These are listed below.

- 1. J. Ray, S. Zeng and N.J. Zabusky Escaped vortex projectiles from shock wave interactions with elliptical and ellipsoidal clouds. Bulletin of the American Physical Society, 42(2) 1109:1109, 1997.
- R. Samtaney, J. Ray and N.J. Zabusky Baroclinic circulation generation on shock accelerated slow/fast gas interfaces. 6TH Int Workshop on Compressible turbulent mixing (IWPCTM): Marseilles 18-21 June 1997, and Phys. Flds, 10(5):1217-1230, 1998.
- N. Zabusky and J. Ray Circulation Deposition and Emergence of Vortex Clusters from Shock-Bubble Interactions. Proceedings of the 2nd International Workshop on Laboratory Astrophysics with Intense Lasers, Univ of Arizona, Tucson, 1998.
- 4. D. Silver and X. Wang, Tracking and Visualizing Turbulent 3D Features, IEEE Trans. on Visualization and Computer Graphics, 3(2), June 1997
- N. Gagvani and D. Silver, Parameter Controlled Skeletonization of Three Dimensional Objects, Technical Report TR-216, CAIP center, Rutgers University, Piscataway, NJ, 1997. Short Paper, Visualization '97 Hot Topics, October 1997.
- N. Gagvani and D. Silver, Parameter Controlled Volume Thinning, submitted for publication, 1998.
- 7. J. Keane, X. Wang, T. Ellman, D. Silver and G. Armhold, Integrated Visualization of Data and Control Flow in Scientific Simulation Programs, Technical Report, Rutgers University.
- 8. X. Wang, D. Silver and K. Ma, Visualizing 4D Features, CAIP Technical Report, October 1997.
- S. M. Zeng and N. Zabusky, Escaped Vortex Projectiles Arising From Strong Shock Wave and Blast Wave Interactions with Spherical Clouds. Bulletin of The American Physical Society, Vo. 41, No. 2, pp. 1109, 1997.
- S.M. Zeng and N. Zabusky, Cavity Collapse and Vortex Projectiles in Shock-Spherical Cloud at High Mach Number Interactions, 6th International Workshop on the Physics of Compressible Turbulent Mixing which will be held in Marseilles, France, June 18-21, 1997
- 11. N. Zabusky and S. M. Zeng, Vortex Projectiles in Shock-Elliptical and Ellipsoidal Bubble Interactions at High Mach Numbers, 6th International Workshop on the Physics of Compressible Turbulent Mixing which will be held in Marseilles, France, June 18-21, 1997.
- 12. J. Ray. R. Samtaney and N. Zabusky, Shock competition and a model for circulation deposition in shock interactions with heavy prolate cylinders Submitted Phys. Flds, 1998.

- 13. Rona, P.A., K.G. Bemis, D.R. Jackson, T. Wen, C. Jones, J.G. Dworski, D.R. Kenchammana-hoskote, and D. Silver, *Acoustic imaging of seafloor hydrothermal flow regimes*, EOS, Trans. Amer. Geophys. Un., 78: F685, 1997.
- 14. P. Rona, K. Bemis, D. Hosekote, D. Silver, Acoustic Imaging and Visualization of Plumes Discharging from Black Smoker Vents on the Deep Seafloor, Case Study, to appear in Proceedings of Visualization '98, October 1998.
- 15. X. Wang and D. Silver, Tracking Features in Unstructured Datasets, to appear in Proceedings of Visualization '98, October 1998.
- 16. N. Gagvani, D. Hosekote, and D. Silver, *Volume Animation*, to appear in Proceedings of Volume Rendering Symposium, October 1998.
- 17. D. Silver, F. Post, A. Sadarjoen, Flow Visualization, to appear in Wiley Encyclopedia of Electrical and Electronics Engineering, 1998.
- 18. X. Wang and D. Silver, Visualizing Evolving Phenomena, to appear in FGCS, 1998.
- R. Samtaney, and J. Ray and N. Zabuksy, Baroclinic circulation generation on shock accelerated slow/fast gas interfaces, Phys. Flds. 10(5):1217-1230, 1998.

6 Conclusion

We are grateful to the AFOSR for this DURIP award.

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